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Approach to the rotation driven vibrational to axially rotational shape phase transition along the yrast line of a nucleus

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Abstract

By analyzing the potential energy surface, the shape phase diagram and the energy spectrum of the nucleus in U(5) symmetry in the IBM, we propose that the U(5) symmetry with parameters $(A + B) < 0$ may be a model to describe the rotation driven vibrational to axially rotational phase transition along the yrast line. With such a model, we have described successfully the observed rotation driven shape phase transition along the yrast line and proposed some other empirical evidences.

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It has been well known that shape phase transition is one of the most significant topics in nuclear structure research. Many evidences of nuclear shape phase transition have been observed. For instance, in several isotopes, there exists shape phase transition from vibration to axial rotation or γ-unstable rotation with respect to the variation of neutron number [1], and a triple point may appear [2,3]. Even in one mode of collective motion there may involve different characteristics, for example, along the yrast line there exists transition between rotations holding different relations between angular momentum and rotational frequency (referred to as band crossing and exhibiting a backbending) [4]. Very recently it was found that there involves rotation driven vibrational to axially rotational shape phase transition along the yrast line of individual nucleus [5]. On the theoretical side, the interacting boson model (IBM) has been shown to be successful in describing the shape phase transition along a series of isotopes [1,6,7]. And analytic solutions for the critical points of the phase transitions have been found [8–10]. The cranked shell model (CSM) [11] has been known to be able to describe the band crossing very well. However, a theoretical approach to describe the rotation driven shape phase transition from vibration to axial rotation along the yrast line in individual nucleus has not yet been established, even though several attempts have been made (see for example Ref. [12]). By analyzing the potential energy surface and the energy spectrum of the U(5) symmetry in the IBM, we will show that the U(5) symmetry with a special choice of parameters can be a model to describe the rotation driven vibrational to axially rotational shape phase transition along the yrast line of individual nucleus.

In the original version of IBM (IBM1), the collective motion of a nucleus is described by the coherent state of s- and d-bosons, which hold angular momentum 0, 2, respectively. The corresponding symmetry group is U(6), and possesses three dynamical symmetry limits, namely, U(5), O(6) and SU(3). With one- and two-body interactions among the

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bosons being taken into account, the Hamiltonian of the U(5) symmetry can be written as [1],

$$\hat{H}_{\mathrm{U}(5)} = E_0 + \varepsilon_d C_{1\mathrm{U}(5)} + A C_{2\mathrm{U}(5)} + B C_{2\mathrm{O}(5)} + C C_{2\mathrm{O}(3)}, \quad (1)$$

where C_{kG} is the k-rank Casimir operator of group G, and the parameters satisfy $C \ll |B| \ll |A| \ll \varepsilon_d$. The IBM may be linked to the collective model of Bohr and Mottelson by implementing the coherent state formalism [1,13–15]. In IBM1, the intrinsic coherent state of a nucleus with N bosons is given by

$$|N;\beta,\gamma\rangle = \left[s^\dagger + \sum_\mu \alpha_\mu d_\mu^\dagger\right]^N |0\rangle, \quad (2)$$

with

$$\alpha_0 = \beta\cos\gamma, \qquad \alpha_{\pm1} = 0, \qquad \alpha_{\pm2} = \frac{1}{\sqrt{2}}\beta\sin\gamma.$$

It is evident that all components of d-bosons can be described by the two parameters β and γ, which have been shown proportional to the deformation parameters in the collective model [1]. For instance, the relations $\hat{\beta}_2 \approx 0.15\beta$ and $\hat{\gamma} = \gamma$ hold for rare earth nuclei, where $\hat{\beta}_2$ and $\hat{\gamma}$ are the quadrupole deformation parameters in collective model. We then refer to the parameters β and γ as deformation parameters in the follows.

It is remarkable that the coherent state of Eq. (2) consists of all possible components of d bosons. As a consequence, it is not an eigenstate of angular momentum, but a superposition of states with all possible values of angular momentum. To investigate the shape phase structure and its transition among the states in ground-state band (or yrast band), we implement the technique of angular momentum projection [16–18] involving projection operator

$$P^L_{MK} = \frac{2L+1}{8\pi^2}\int D^L_{MK}{}^*(\Omega)R(\Omega)\,d\Omega, \quad (3)$$

with $M = K = 0$. Then the energy functional (i.e., potential energy surface) of the state with angular momentum L in the ground-state band can be given as

$$E_{\mathrm{gsb}}(N,L,\beta,\gamma) = \frac{\langle N;\beta,\gamma|\hat{H}P^L_{00}|N;\beta,\gamma\rangle}{\langle N;\beta,\gamma|P^L_{00}|N;\beta,\gamma\rangle}. \quad (4)$$

With the rotation operator written explicitly, Eq. (4) becomes

$$E_{\mathrm{gsb}}(N,L,\beta,\gamma) = \frac{\int_0^\pi d\beta'\sin\beta' d^L_{00}(\beta')\langle N;\beta,\gamma|\hat{H}e^{-i\beta' J_y}|N;\beta,\gamma\rangle}{\int_0^\pi d\beta'\sin\beta' d^L_{00}(\beta')\langle N;\beta,\gamma|e^{-i\beta' J_y}|N;\beta,\gamma\rangle}, \quad (5)$$

where $d^L_{mm'}(\beta')$ is the reduced rotation matrix.

After some derivations, and considering that the deformation parameter β should be rather small for the vibrational to axially rotational ($\gamma = 0$) shape phase transition of current interest, we can approximate the potential energy surface of Eq. (5) up to β^6 as

$$E_{\mathrm{gsb}}(N,L,\beta) = A_0 + \frac{1}{2}\alpha(L-L_0)\beta^2 + \frac{1}{4}A_4\beta^4 + \frac{1}{6}A_6\beta^6, \quad (6)$$

with

$$A_0(N,L,\varepsilon_d,A,B,C) = \frac{1}{4}\big[2\varepsilon_d + 8A + 6B + 4C + (A+B+4C)L\big]L,$$

$$\alpha = \frac{L(2N-L)(A+B)}{2(3+2L)},$$

$$L_0 = \frac{\varepsilon_d + 5A + 4B}{-(A+B)}.$$

A_4 and A_6 are also functions of the interaction parameters ε_d, A, B, C and the state indices N, L.

It follows from the spectrum generating principle that $L \in [0, 2N]$, $\varepsilon_d > 0$, while A, B and C may be either positive or negative. If $(A+B) > 0$, then $\alpha > 0$ and $L_0 < 0$, so that $\alpha(L-L_0)$ remains positive. Otherwise, if $(A+B) < 0$ (the dynamical symmetry condition guarantees $(\varepsilon_d + 5A + 4B) > 0$), then $\alpha < 0$ and $L_0 > 0$, so that $\alpha(L-L_0)$ may change from positive to negative as the angular momentum L increases from under to over L_0. Because of the complexity of the A_4 and A_6 in terms of the parameters N, L, ε_d, A, B and C, it is difficult to discuss the variation characteristics analytically. Numerical calculation indicates that, when the parameters in the Hamiltonian are taken as $\varepsilon_d > 0$, $(A+B) < 0$ and $C > 0$, the parameters A_4, A_6 in Eq. (6) can be negative, positive, respectively. It becomes then evident that the energy functional of Eq. (6) closely resembles the Landau free-energy [19,20] in the theory of thermodynamic phase transition, with L and β playing the roles of control parameter and order parameter, respectively.

A more quantitative analysis is now in order for the potential energy surface of Eq. (6). If the parameters in the Hamiltonian (1) are chosen as $(A+B) > 0$, we have $\frac{\partial^2 E_{\mathrm{gsb}}(N,L,\beta)}{\partial\beta^2}|_{\beta=0} = \alpha(L-L_0) > 0$. Then the potential energy is minimized only at $\beta = 0$. The nucleus with such a potential energy functional would always stay in a vibrational shape phase. If $(A+B) < 0$, then $\alpha < 0$ and $L_0 > 0$, so $\frac{\partial^2 E_{\mathrm{gsb}}(N,L,\beta)}{\partial\beta^2}|_{\beta=0} > 0$ for $L < L_0$, and $\frac{\partial^2 E_{\mathrm{gsb}}(N,L,\beta)}{\partial\beta^2}|_{\beta=0} < 0$ for $L > L_0$. The point $\beta = 0$ evolves from a local minimum to a local maximum of the potential energy surface when L rises from below to above L_0. Furthermore, there exists a critical angular momentum $L_c = L_0 + \frac{3A_4^2}{16A_6\alpha}$, with which the energy surface acquires two and equal minima at $\beta = 0$ and $\beta = \sqrt{-3A_4/4A_6}$, respectively. There is another critical value $L_{\max}$ for the angular momentum, beyond which a nucleus becomes unstable as the energy functional is no longer lower-bounded. It follows from Eq. (6) that $L_{\max} = 2N$, the highest angular momentum possible, when $A_6 > 0$, whereas $L_{\max} = L_0 + \frac{A_4^2}{4A_6\alpha}$ when $A_6 < 0$. In any case, we have $L_{\max} > L_0$. For the states with $L \in (L_c, L_{\max}]$, the energy functional is maximized at $\beta = 0$ and minimized at some $\beta \neq 0$. As already mentioned, the energy functional has no minimum for the states with angular momentum $L \in (L_{\max}, 2N]$. The β-dependence of the energy surface for some typical values of angular momentum L is illustrated in Fig. 1, where L_0 and L_c are calculated as 8 and 6, respectively. It becomes apparent that a nucleus has a stable vibrational shape phase with states around $\beta = 0$, if the

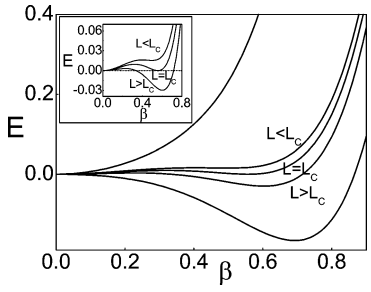


Fig. 1. The energy surface (Landau free energy) of a nucleus against the "deformation parameter" β at some typical angular momentum L (with the parameters in Eq. (1) being taken as $\varepsilon_d = 1.010812$ MeV, $A = -0.153669$ MeV, $B = 0.0822402$ MeV, $C = 0.0185084$ MeV).

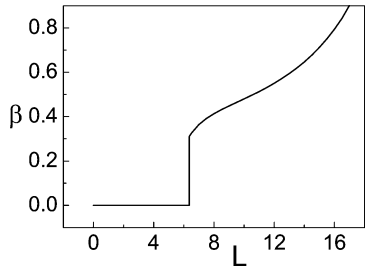


Fig. 2. The vibration and rotation phase diagram of a nucleus in terms of the angular momentum L and the "deformation parameter" β (with the same parameters for Fig. 1).

Hamiltonian parameter $(A + B) < 0$ and the angular momentum $L < L_c$. In the regime of $L \in (L_c, L_{\max}]$, the only stable shape phase is rotational with states around the energy minimum at some $\beta \neq 0$. For $L = L_c$, the energy surface has two degenerate but distinct minima, one of which is localized at $\beta = 0$, the other is localized at some $\beta \neq 0$. Under such a condition, the system may undergo a transition from one energy minimum to the other, and when that happens, the symmetry of the system is spontaneously broken. Such transition is of the first order, according to the standard theory of phase transition. The same theory would also predict the coexistence of vibrational and rotational shapes with $L = L_c$ as a precursor of a shape phase transition [21,22]. When the angular momentum $L > L_{\max}$, a nucleus may not be able to maintain a stable structure. Fig. 2 depicts the shape phase diagram of a nucleus in terms of the angular momentum L and the deformation parameter β, where the same interaction parameters as in Fig. 1 are used, L_0 and L_c still are 8 and 6, respectively.

The above discussion has shown explicitly that the potential energy functional derived from the U(5) symmetry with $(A + B) < 0$ has the similar mathematical form of the Landau free-energy [19,20], which puts a U(5)-symmetric nuclear system in the standard theoretical framework of first-order phase transition, so to correctly predict and well describe the vibrational to axially rotational nuclear shape phase transition in the ground-state band (or along the yrast line).

On the phenomenological side, the energy spectrum of a nucleus in U(5) symmetry can be given as

$$E_{\mathrm{U}(5)} = E_0 + \varepsilon_d n_d + A n_d(n_d + 4) + B\tau(\tau + 3) + C L(L + 1), \tag{7}$$

where n_d, τ, and L are the irreducible representations (IRREPs) of the group U(5), O(5) and O(3), respectively.

From the spectrum generating process one can recognize that, if $A > 0$ and $B > 0$, the states with $\tau = n_d$, $L = 2n_d$ form the ground state band and simultaneously the yrast band, and the energy of the state in the ground state band can be given as

$$E_{\mathrm{gsb}}(n_d) = E_0 + (A + B)n_d^2 + (\varepsilon_d + 4A + 3B)n_d + C L(L + 1).$$

The energy spectrum appears as the anharmonic vibrational one with increasing frequency $\hbar\omega = (\varepsilon_d + 4A + 3B) + (A + B)n_d$ (if the anharmonic effect induced by the rotation is taken into account, the vibrational frequency increases with n_d in the relation $\hbar\omega = (\varepsilon_d + 4A + 3B + 2C) + (A + B + 4C)n_d$). However, if $(A + B) < 0$, the $E_{\mathrm{gsb}}(n_d)$ $(E_{\mathrm{gsb}}(L))$ is an upper-convex parabola against the n_d (L) and appears as the anharmonic vibrational one with decreasing frequency. From these anharmonic vibrational characteristics, one can recognize that, when $(A + B) < 0$, there exists a d-boson number $n_d^{(c)}$ and an angular momentum

$$L_c = 2n_d^{(c)} = -\frac{2(\varepsilon_d + 4A + 3B)}{A + B} - 2N_0, \tag{8}$$

where $N_0 = N$ with N being the total boson number. As the angular momentum $L \geqslant L_c$, the yrast states are no longer the anharmonic vibrational ones mentioned above, but the quasi-rotational ones with $n_d = N_0$. Recalling the analysis in the coherent state formalism with angular momentum projection, one can conclude that the U(5) symmetry with parameters $(A + B) < 0$ can describe the vibrational to axially rotational shape phase transition along the yrast line. The L_c given in Eq. (8) is the critical angular momentum. For each yrast state with angular momentum $L < L_c$, its energy can be given as

$$E(L < L_c) = E_0 + \frac{A + B + 4C}{4}L^2 + \frac{\varepsilon_d + 4A + 3B + 2C}{2}L. \tag{9}$$

Whereas for the one with angular momentum $L \geqslant L_c$, its energy should be expressed as

$$E(L \geqslant L_c) = E_0' + C L(L + 1), \tag{10}$$

and can be displayed as a part of an upper-concave parabola. For instance, for a system with $N = 15$ and parameters $\varepsilon_d = 0.80$ MeV, $A = -0.025$ MeV, $B = -0.01$ MeV and $C = 0.004$ MeV, with Eq. (8) we can fix the critical angular momentum $L_c = 8\hbar$. The energy of the yrast states against the angular momentum L can be illustrated in the left panel of Fig. 3. It has been known that the energy of E2 transition γ-ray over spin (E-GOS) $R = \frac{E_\gamma(L \to L-2)}{L}$ can be taken as a quite good signature to manifest the vibrational to axially rotational phase transition along the yrast line [5]. As an auxiliary evidence, we show also the E-GOS of the yrast states with above parameters in the right panel of Fig. 3. The figure indicates apparently that the yrast states involve a vibrational to axially rotational phase transition and the angular momentum L_c is definitely the critical point for the phase transition to take place. Such a transition is quite similar to that between the states with $n_p = 0$ and $n_p = N$ [23] in the vibron model [24] with random interactions.

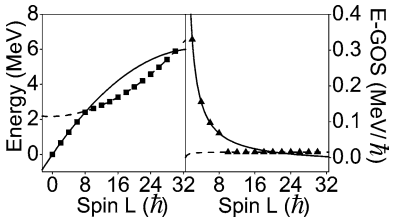


Fig. 3. An example of the energy against spin (left panel) and the E-GOS (right panel) along the yrast line (filled squares and triangles, respectively) in the approach of U(5) symmetry with $(A+B)<0$ (with parameters $\varepsilon_d = 0.80$ MeV, $A = -0.025$ MeV, $B = -0.01$ MeV, $C = 0.004$ MeV. The solid and dashed lines are implemented to guide the eye).

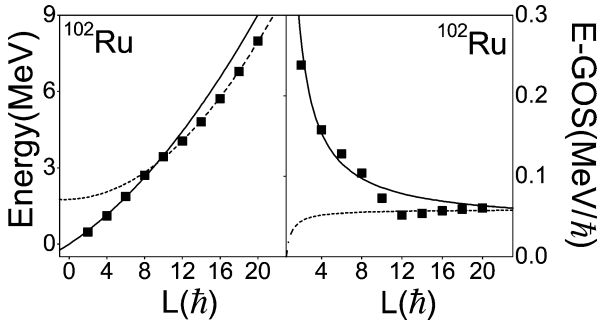
Table 1
Fitted parameters of the bands ^{102}Ru, ^{112}Cd, ^{114}Cd, ^{114}Te, ^{142}Sm and ^{188}Hg

Band	ε_d (MeV)	A (MeV)	B (MeV)	C (MeV)	N	L_c
^{102}Ru	0.5281	−0.009376	−0.008819	0.01475	20	12
^{112}Cd	0.6581	−0.007640	−0.01327	0.01440	25	10
^{114}Cd	0.5695	−0.0003789	−0.01586	0.01393	29	10
^{114}Te	0.7747	−0.01678	−0.01423	0.01269	17	12
^{142}Sm	1.101	−0.06263	−0.01165	0.01713	7	10
^{188}Hg	0.5957	−0.03057	−0.002976	0.009193	9	12

Reviewing above analysis, one knows that, in the anharmonic vibrational model, there involves competition between vibration and rotation. In the case of that the interaction parameters are taken as $(A+B)<0$, the vibrational frequency decreases and the rotational effect increases if the angular momentum (or d boson number) increases. As the angular momentum L (or n_d) reaches the critical value, the vibration disappears, so that only the rotational effect governs the property of state. Simultaneously, a sudden increase happens in the d boson number. Then the structure of the wavefunction changes from the vibrational one to the rotational one, so that the vibrational to the axially rotational shape phase transition takes place. In the microscopic point of view, cranking random phase approximation calculation has shown that the gradual decrease of vibration can induce a backbending, i.e., a shape phase transition [25]. On phenomenological level, the U(5) symmetry with parameter $A<0$ has been used to describe the collective backbending of high spin states successfully [26].

As an application of our presently proposed model, we analyze the typical example ^{102}Ru involving the rotation driven vibrational to axially rotational shape phase transition [5]. By fitting the experimental data of the yrast band of ^{102}Ru with Eqs. (9) and (10), we obtain the energy spectrum and the E-GOS plots as shown in Fig. 4. To show the sudden change of the wavefunction, we also list the configuration (n_d, τ, L) of the sates in the yrast band in Fig. 4 and the fitted parameters in Table 1. Fig. 4 and Table 1 show evidently that the shape phase transition happens at angular momentum $L = 12$ and our model describes well such a shape phase transition.

We have also analyzed the available experimental energy spectra of the yrast bands of even–even nuclei with $30 \leqslant Z \leqslant 100$ and simulated the data with least-square fitting in our present model. We find that, besides the yrast bands of nuclei ^{102}Ru, ^{112}Cd and ^{114}Cd identified by Regan and collaborators



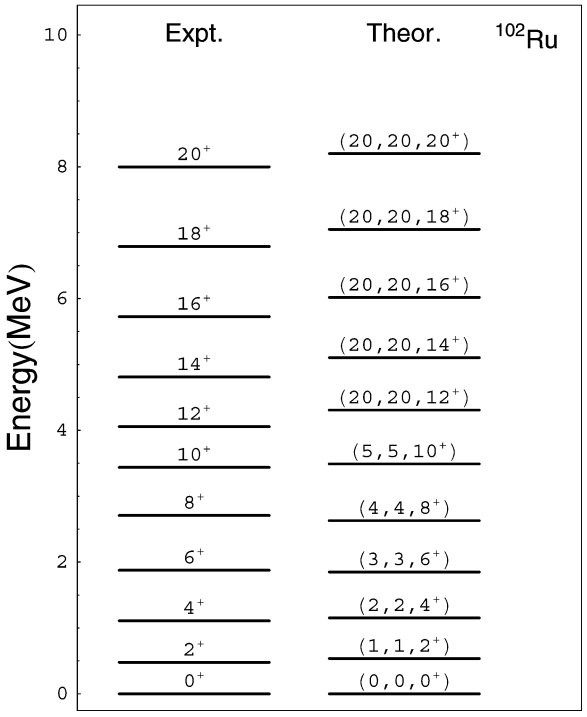


Fig. 4. The theoretically obtained energy spectrum and E-GOS plot of the yrast band of ^{102}Ru (curve) and the comparison with experimental data (filled squares, taken from Ref. [5]).

in Ref. [5], the yrast bands of nuclei ^{114}Te, ^{142}Sm and ^{188}Hg involve the vibrational to axially rotational shape phase transition. The theoretical results of the energy spectra and the E-GOS plots of these bands and the comparison with experimental data are illustrated in Fig. 5. The fitted parameters are listed in Table 1. From Fig. 5 and Table 1, one can infer that our model can describe the rotation driven shape phase transition successfully.

Looking over the fitted boson number listed in Table 1, one may know that, for ^{142}Sm and ^{188}Hg, it agrees well with the simple ansatz: boson number is half of the valence nucleons (or holes). However, for the nuclei in $A \sim 110$ mass region, it differs from half of the valence nucleons obviously. Recalling the recent suggestion that the valence neutrons may be in the $h_{11/2}$ orbital [5,27], we infer that the microscopic configuration of the nuclei in $A \sim 110$ mass region is so complicated that the boson number of them cannot be simply taken as half of the valence nucleons. It means that the effective boson number may be important to the structure of these nuclei. In fact, quite early

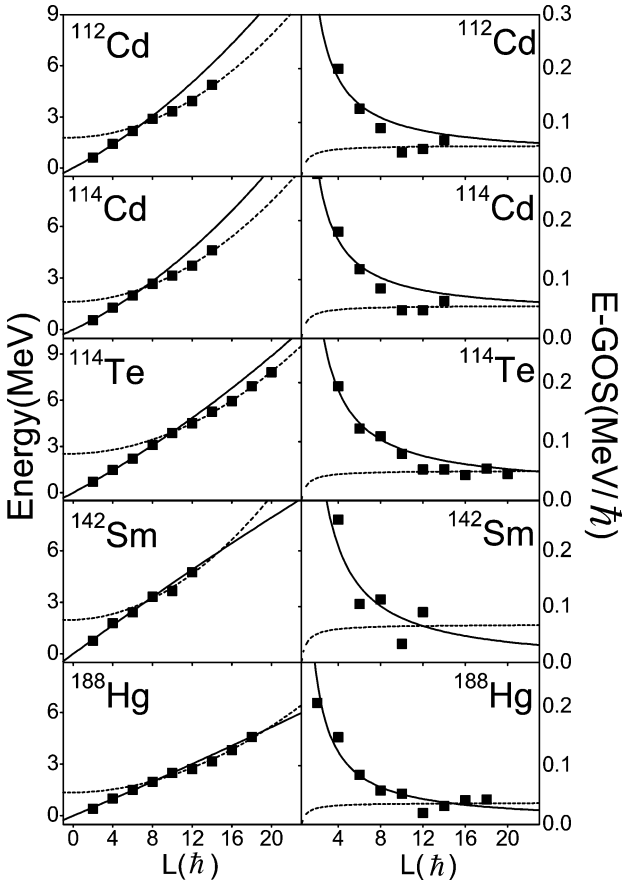


Fig. 5. The theoretically obtained energy spectrum and E-GOS plot of the yrast bands of ^{112}Cd, ^{114}Cd, ^{114}Te, ^{142}Sm and ^{188}Hg (curve) and the comparison with experimental data (filled squares, taken from Refs. [32–35]).

IBM calculations [28–31] had shown that, to describe the spectroscopic property of these nuclei well, effective boson number should be implemented. Then we believe that the fitted boson number is reasonable, even though it is not consistent with half of the valence nucleons for the $A \sim 110$ nuclei. Meanwhile it provides a clue that the structure of the nuclei involving rotation driven vibrational to axially rotational shape phase transition is very complicated and needs sophisticated investigation.

In summary, by analyzing the potential energy surface of the nucleus in U(5) symmetry in the coherent state formalism with angular momentum projection in the IBM, we give a phase diagram of the vibration and the rotation in terms of the angular momentum and the deformation parameter in this Letter. We have then proposed that the U(5) symmetry with parameters $(A + B) < 0$ may be a model to describe the rotation driven vibrational to axially rotational shape phase transition along the yrast line. With such a model, we have described successfully the vibrational to axially rotational phase transition along the yrast line in $A \sim 110$ mass region identified by Regan and collaborators [5]. By analyzing the available experimental spectra of even–even nuclei with $30 \leqslant Z \leqslant 100$, we show that, besides the ones in $A \sim 110$ mass region, the yrast band of nuclei ^{114}Te, ^{142}Sm and ^{188}Hg may also be the empirical evidences involving the rotation driven vibrational to axially rotational shape phase transition.

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